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Final Report: Parallel Multi-Scale Algorithms and Applications to Turbulence

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Objectives

Support for one graduate was awarded to augment the numerical and computational work performed under AFOSR Grants F49620-94-1-0313 and F49620-97-1-0185 in the Computational Mathematics Program. In particular, we developed and implemented parallel algorithms for computational electromagnetics with applications to turbulence control, and new algorithms for velocity-vorticity formulations appropriate for high Reynolds number flows. These algorithms are based on the multiscale spectral discretizations for unstructured meshes we developed in the parent grants. The implementation was performed on the IBM SP2 and SP3 at Brown University and MHPCC as well as on different parallel platforms, including Linux clusters, using the MPI communications protocol.

1 Research Project Description

We developed a new hierarchical spectral basis appropriate for hp-finite element formulations on unstructured and hybrid grids consisting of tetrahedral, prismatic and pyramidal subdomains. This unique basis is the building block for the accurate (spectral) solution of partial differential equations in complex geometry computational domains. An important feature of this work is that high-order accuracy can be obtained on standard unstructured and hybrid CFD meshes. Moreover, unlike low-order discretizations which may require Delaunay triangulations for convergence, the new hierarchical basis can be used in conjunction with highly distorted meshes without accuracy degradation.

The accuracy of the new method was tested both in two- and three-dimensions for benchmark Navier-Stokes and MHD equations. For smooth solutions we obtained exponential convergence irrespective of the grid distortion. Based on this new formulation a flow solver (NEKTAR) was developed in order to be used in turbulence and MHD simulations. There are three important new features of this code that make it superior to our previous spectral element flow solvers:

- First, it is fully adaptive as h- and p-type refinement can be readily applied using the hierarchical structure of the basis. For example, each edge or face or the interior in each tetrahedron could have different modes according to resolution demands.
- Second, it is more efficient as more effective preconditioners can be constructed

using multi-resolution type algorithms. These discretizations has also been employed to solve the magneto-hydrodynamics (MHD) equations as described in the original proposal.

- Third, the development of Discontinuous Galerkin projections. This is a *break-through* in variational numerical methods, which may have great impact in many AFOSR applications. It allows general high-order differential operators to be discretized with finite jumps (L^2 continuity) across subdomains. This, in turn, implies that “sliding” domains (of great interest to weapons simulation technology) can now be discretized with no extra computational effort.

The specific tasks completed are:

- **NEKTAR-MHD simulation code:** For fully three-dimensional geometries we extended our base code **NEKTAR**, that allows for spectral discretizations on three-dimensional unstructured meshes consisting of tetrahedra or other subdomains, to include the MHD formulation described previously. Validation includes comparisons with exact solutions such as the three-dimensional Hartmann-Hunt solution as well as comparisons with numerical solutions from our validated code **PRISM**.
- **Electro-Magnetic Flow Control:** Here we employed the NEKTAR-MHD code to examine different combinations of electric and magnetic fields for suppressing near-wall turbulence fluctuations. Experimental evidence suggests that the direction of the resultant Lorentz force is very important with the largest drag reduction produced with a force normal to the wall. This finding was studied in detail in simulations using slightly conducting fluids such as ionized gas and salt water, leading eventually to a publication in *Science*, May 2000.

- **Velocity-Vorticity Penalty Formulation:**

The objective of this task was to develop a parallel vorticity-velocity spectral element method for the incompressible Navier-Stokes equations to study turbulence in complex geometries. To understand why the vorticity-velocity spectral element method is chosen, consider the problem of high Reynolds number flow past a cylinder. Vorticity dynamics plays a crucial role in the separation of the boundary layer and the three-dimensionality in the wake. The boundary layer forming around the cylinder is proportional to $Re^{-\frac{1}{2}}$. At the surface of the cylinder, vorticity is created in the boundary layer and shed into the wake.

Since it is necessary that at least a few mesh points are in the boundary layer, the condition that $\delta Re \sim \mathcal{O}(1)$ must be satisfied where δ is mesh width. As a result, one of the difficulties of simulating high Reynolds number flows is the number of mesh points is large and hence the computational effort is prohibitively large. Another major difficulty is knowing the amount of vorticity created at the boundary.

A new parallel three-dimensional vorticity-velocity formulation was developed based on a rigorous equivalence theorem. The vorticity-velocity formulation is based on a semi-implicit temporal discretization and the spectral element spatial discretization. The penalty method based on the semi-discrete equations is the key to imposing high-order accurate vorticity boundary conditions. A distinction of the formulation presented here is that the vorticity and velocity fields are expanded in the same discrete space (polynomial order), while other low order finite element vorticity-velocity formulations expand the vorticity in a subspace of lower order than the velocity. The penalty vorticity boundary conditions are imposed by augmenting the weak Galerkin formulation of the vorticity transport equation at the boundary.

- **Computational Steering Environment:**

We developed a new computing approach in simulation, namely *computational steering*, where the developed hierarchical spectral methods are used on grids changing continuously in time by following an adaptive procedure. We have developed and performed such computational steering procedures for parallel computers in conjunction with interactive graphics in order to introduce a new mode of Direct Numerical Simulation, i.e. the *dynamic DNS*, *dDNS*.

Personnel

- Faculty: G.E. Karniadakis (US), Professor of Applied Mathematics.
- PhD Students: J. Trujillo (US citizen, minority) and R.M. Kirby (US citizen).

Publication

1. J. Trujillo, "Effective high-order vorticity-velocity formulation", PhD thesis, Princeton University, 1998 (supervised by the PI).

2. T.C. Warburton, "Spectral/hp Methods on Polymorphic Multi-Domains: Algorithms and Applications", PhD thesis, Brown University, 1998 (supervised by the PI).
3. C. Evangelinos, S.J. Sherwin and G.E. Karniadakis, "Parallel DNS algorithms on unstructured grids", C.M.A.M.E., vol. 184, pp. 401-425, (2000).
4. R.M. Kirby, T.C. Warburton, I. Lomtev and G.E. Karniadakis, "A discontinuous Galerkin spectral/hp method on hybrid grids", Applied Numerical Mathematics, vol. 33, pp. 393-405, (2000).
5. J. Trujillo and G.E. Karniadakis, "A penalty method for the vorticity-velocity formulation", J. Comp. Phys., vol. 149, pp. 32-58, (1999).
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7. T.C. Warburton, S.J. Sherwin and G.E. Karniadakis, "Basis functions for triangular and quadrilateral high-order elements", SIAM J. Scientific Computing, vol. 20 (5), pp. 1671-1695, (1999).
8. G.S. Karamanos, C. Evangelinos, R. Boes, R.M. Kirby and G.E. Karniadakis, "DNS of turbulence on a PC/Linux cluster: Fact or Fiction?", Proc. Super-Computing 1999.
9. S.J. Spencer, T.C. Warburton, and G.E. Karniadakis, "Spectral/hp methods for elliptic problems on hybrid grids", Contemporary Mathematics, vol. 218, p. 191-215, 1998.
10. C.H. Crawford and G.E. Karniadakis, "Reynolds Stress Analysis of EMHD-controlled Wall Turbulence, Part I: Streamwise Forcing", Phys. Fluids, vol. 9(3), p. 788, 1997.
11. C.H. Crawford and G.E. Karniadakis, "Reynolds stress analysis of controlled wall-turbulence", AIAA 96-2008, 27th AIAA Fluid Dynamics Conference, June 17-20, New Orleans, LA, 1996 (invited paper).
12. C.H. Crawford, C. Evangelinos, D.J. Newman and G.E. Karniadakis, "Parallel Computations of Turbulence in Complex Geometries", Computer & Fluids, vol. 9, p. 273, 1996.

Interactions/Transitions

The two students funded by AASERT, J. Trujillo and R. M. Kirby, attended every year the APS Fluid Dynamics meeting and presented results related to this grant. In addition, the PI (Karniadakis) was invited to present the AFOSR-sponsored research at:

• MIT • Cornell Theory Center • Boston University • Virginia Polytechnic Institute • Hong Kong University • International Conference on Parallel Algorithms and Applications (Wuhan, China) • Institute for Scientific Computing, Chinese Academy of Sciences • Institute of Mechanics, Chinese Academy of Sciences • University of Tokyo • University of Notre Dame • University of California Santa Barbara • Wright Patterson Air Force Base • City College/Levich Institute • AFOSR Boiling AFB DC • Nuclear Regulatory Commission • National Institute of Standards and Technology • AIAA Conference New Orleans • Cornell Workshop on POD-Galerkin Models • University of Michigan • AFOSR/Princeton • DARPA/NUWC Workshop on EMTC • DOE/Oakridge Workshop on DGM • NSF Workshop • AIAA Fluid Dynamics Conference on LES • SIAM Annual Meeting/Symposium on MHD • ICOSAHOM'98 Symposium • Japanese Society of Fluid Mechanics 30th Anniversary Symposium • University of Tokyo • Turkey Workshop on Industrial and Environmental Applications of DNS/LES • Caltech Symposium on Validation and Verification; • Argonne National Labs • Boston University • Los Alamos National Laboratory • University of Texas A & M • American Physical Society •

The code NEKTAR is an open source code, and it has been distributed to more than two dozen Universities and Laboratories. Some of them include AFB Research Lab at Kirkland, Boeing, MIT, Berkeley, Caltech, Cornell University, Penn State University, University of Wisconsin, Imperial College, North Carolina University, Florida State University, OAK Ridge Labs, Nielsen, Inc., etc. There is limited documentation of the code, which has made this distribution somewhat difficult.